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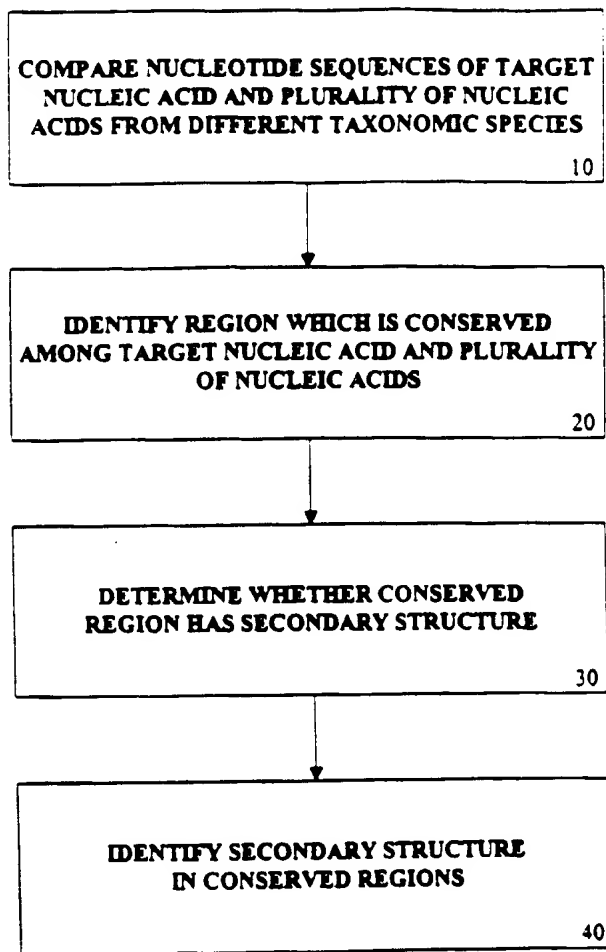


FIGURE 1

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Find Neighbors  
and Assemble  
Flow Diagram

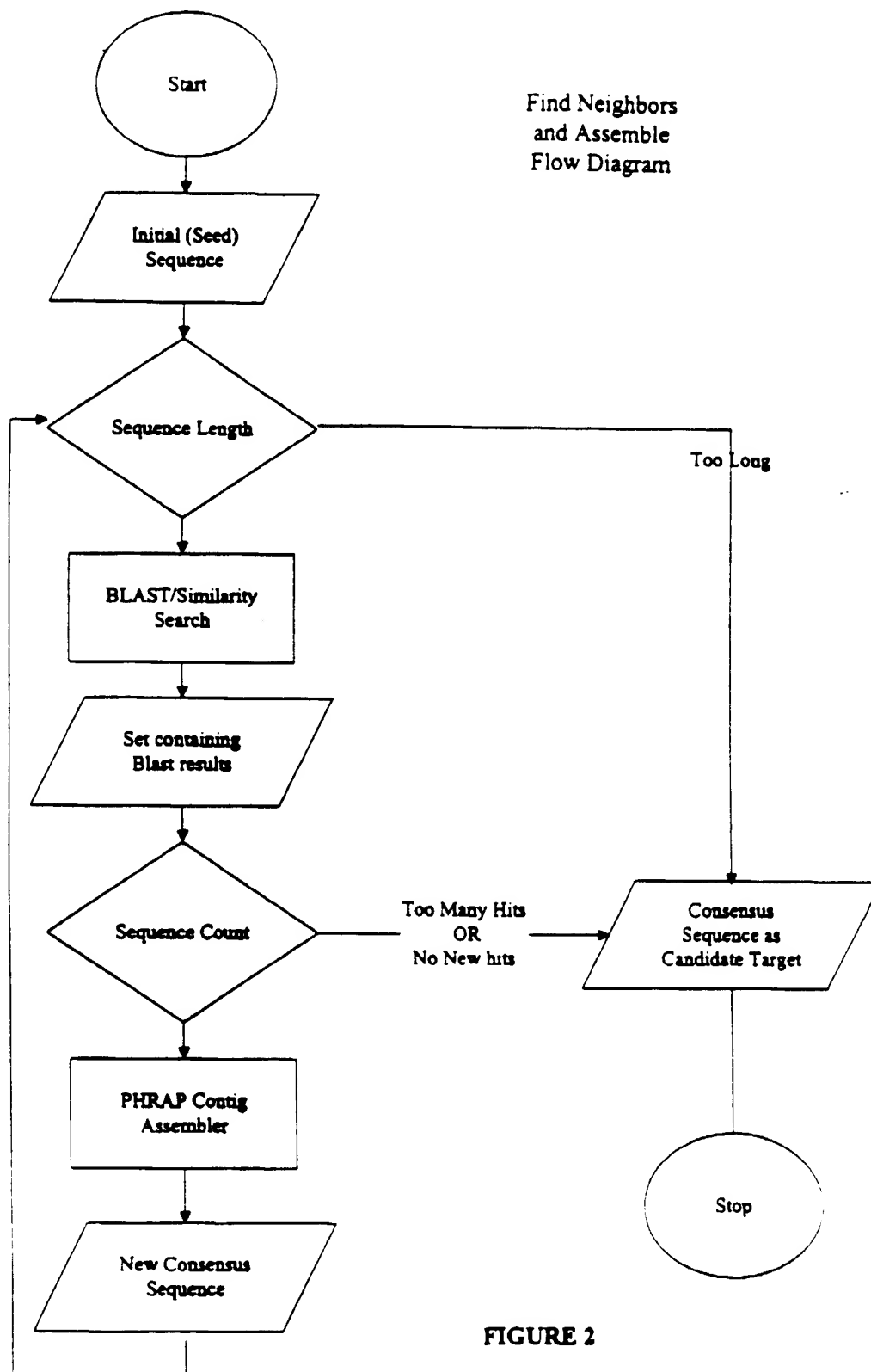


FIGURE 2

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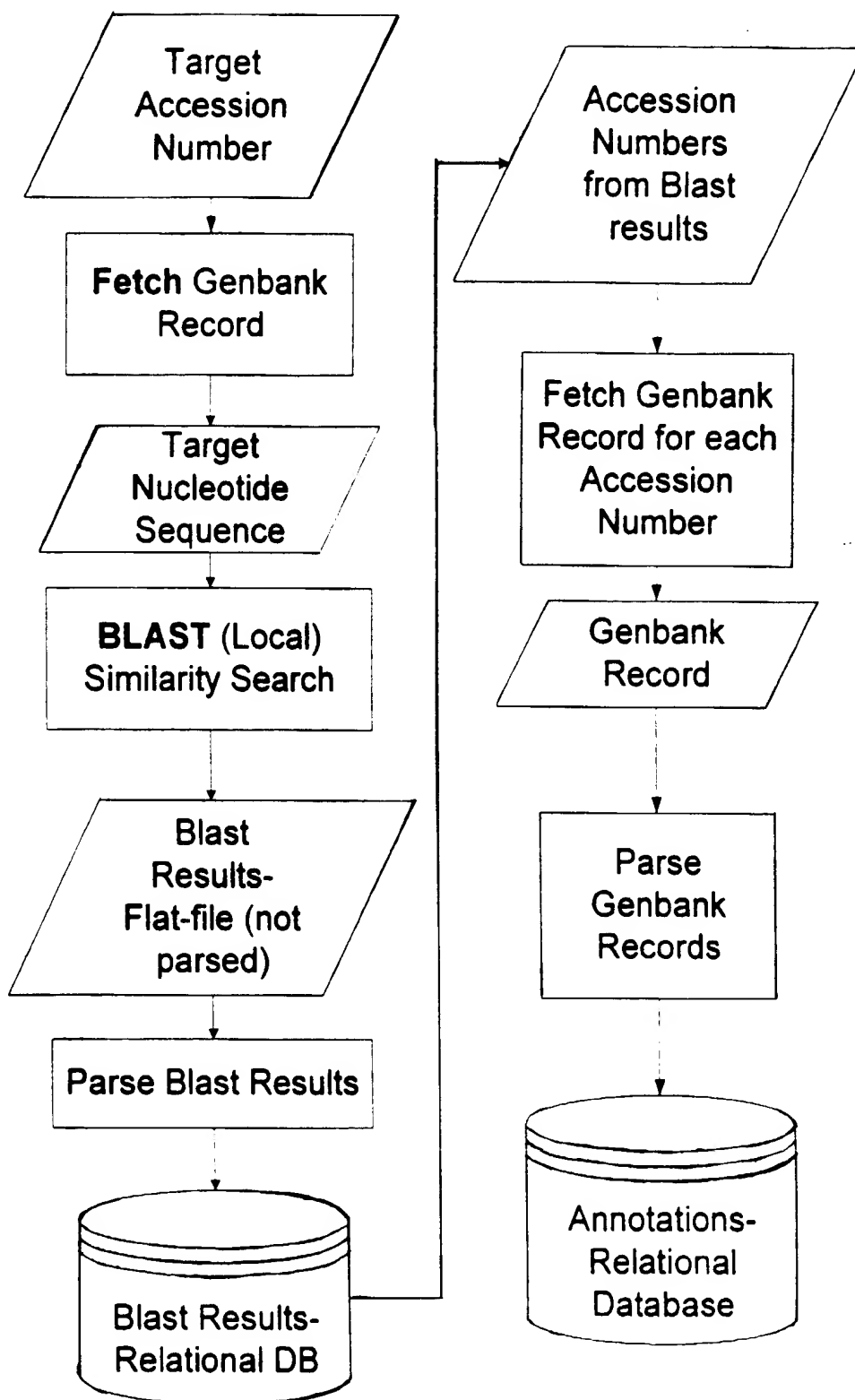


Figure 3

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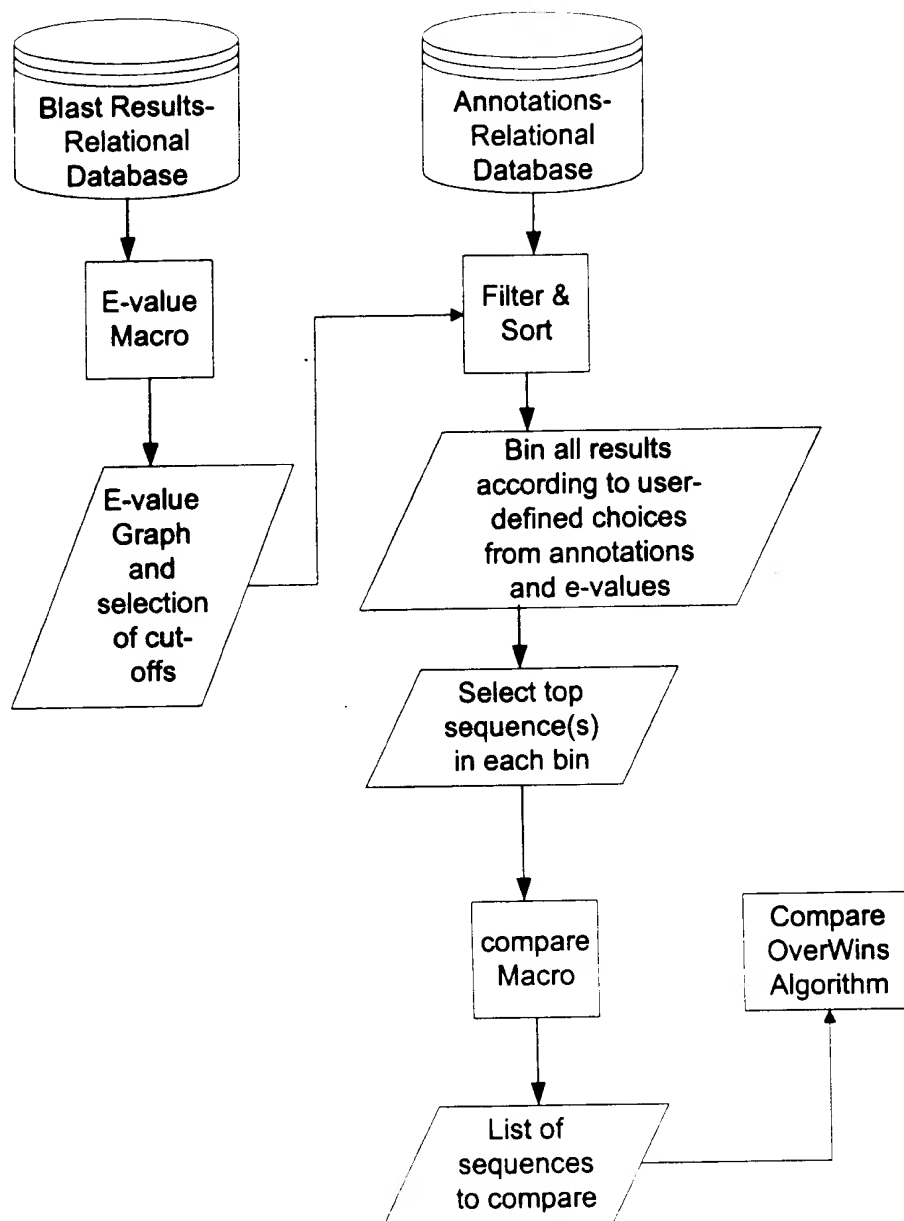
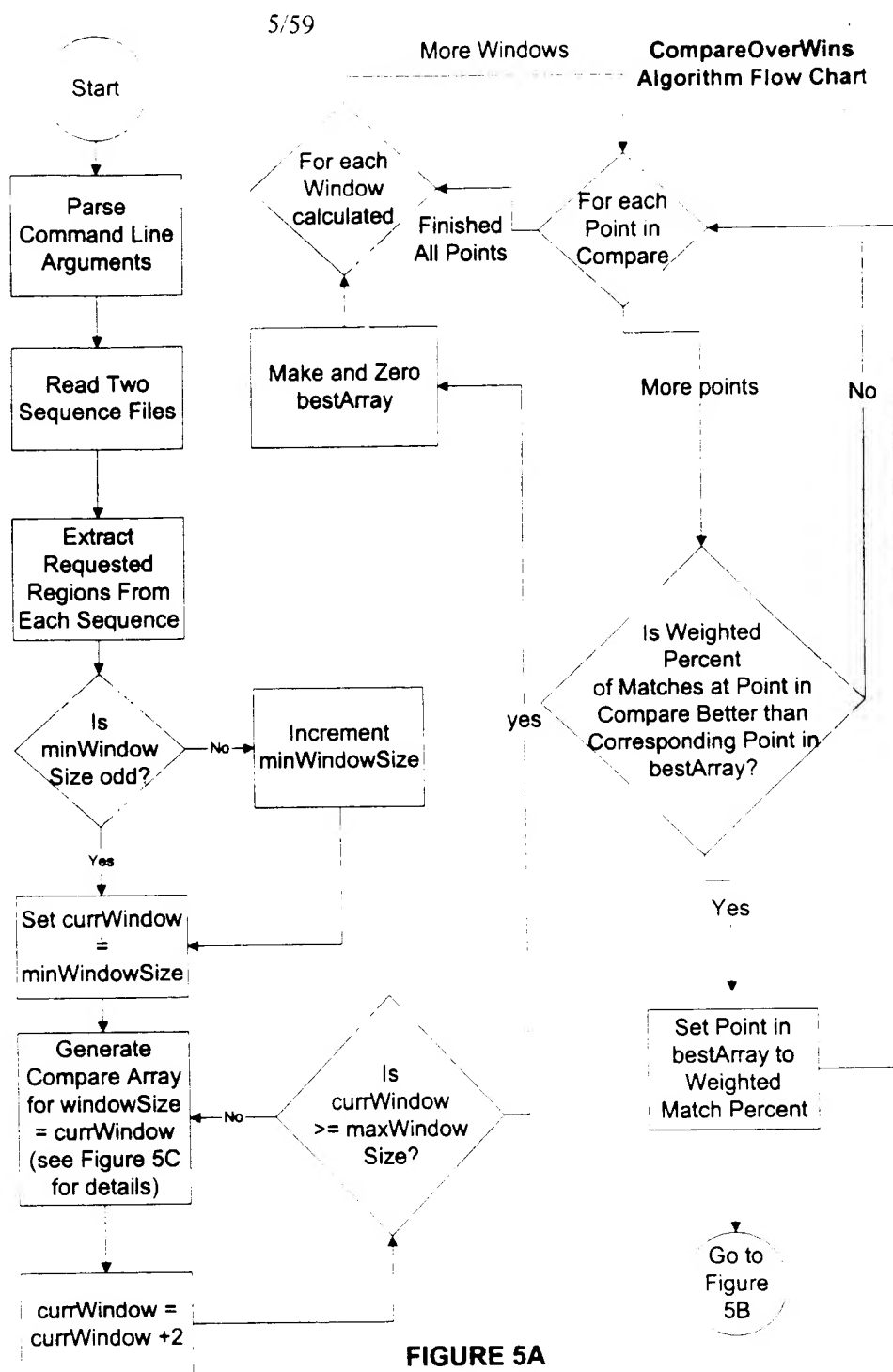


FIGURE 4



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# CompareOverWins Algorithm Flow Chart

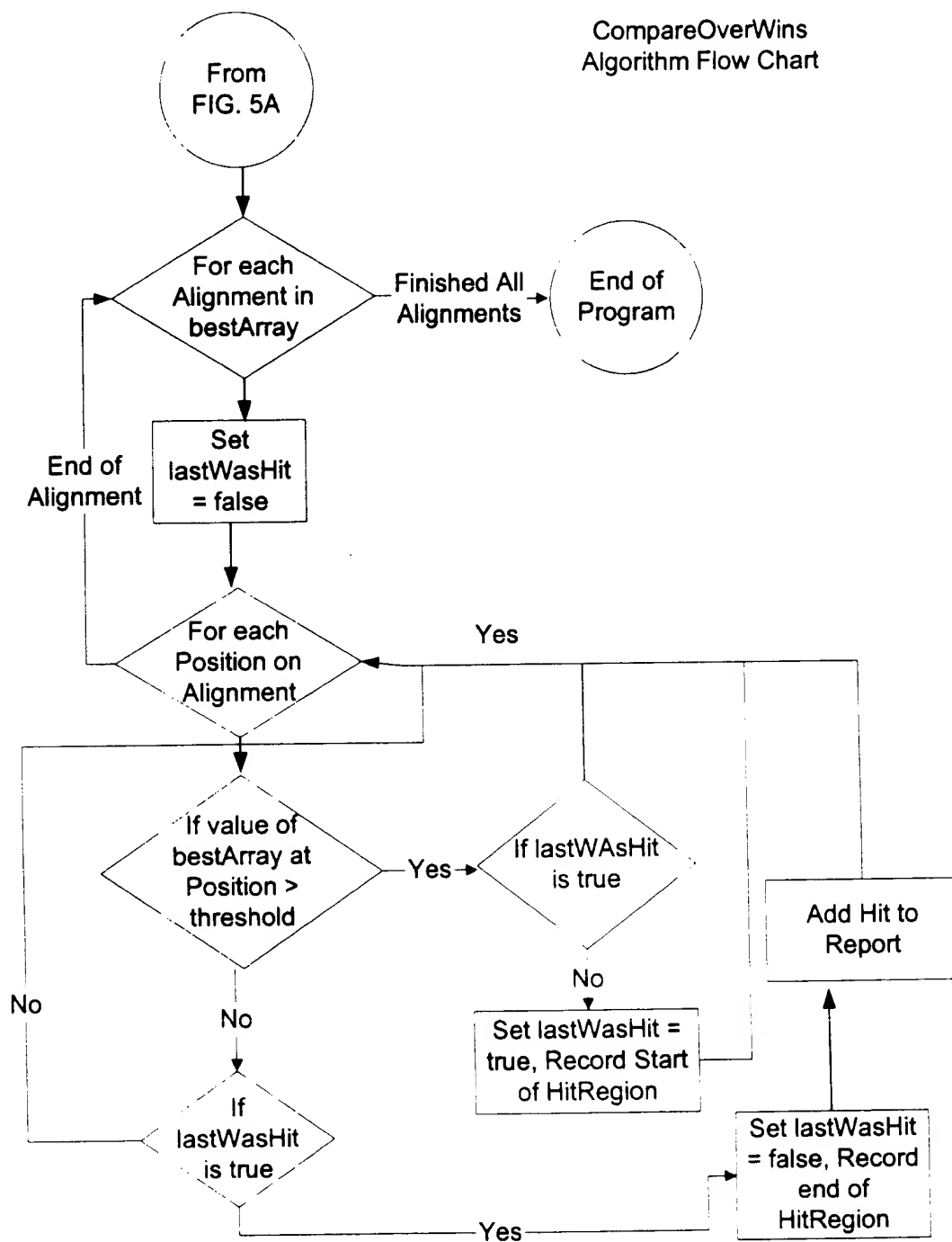


FIGURE 5B

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Input:  
 Sequence A length a  
 Sequence B length b  
 Window Size

# CompareOverWins Algorithm Flow Chart Basic Compare

Output:  
 Array of size a by b of unsigned chars (0-255)  
 Each point represents the number of matches in the  
 window at that alignment and position

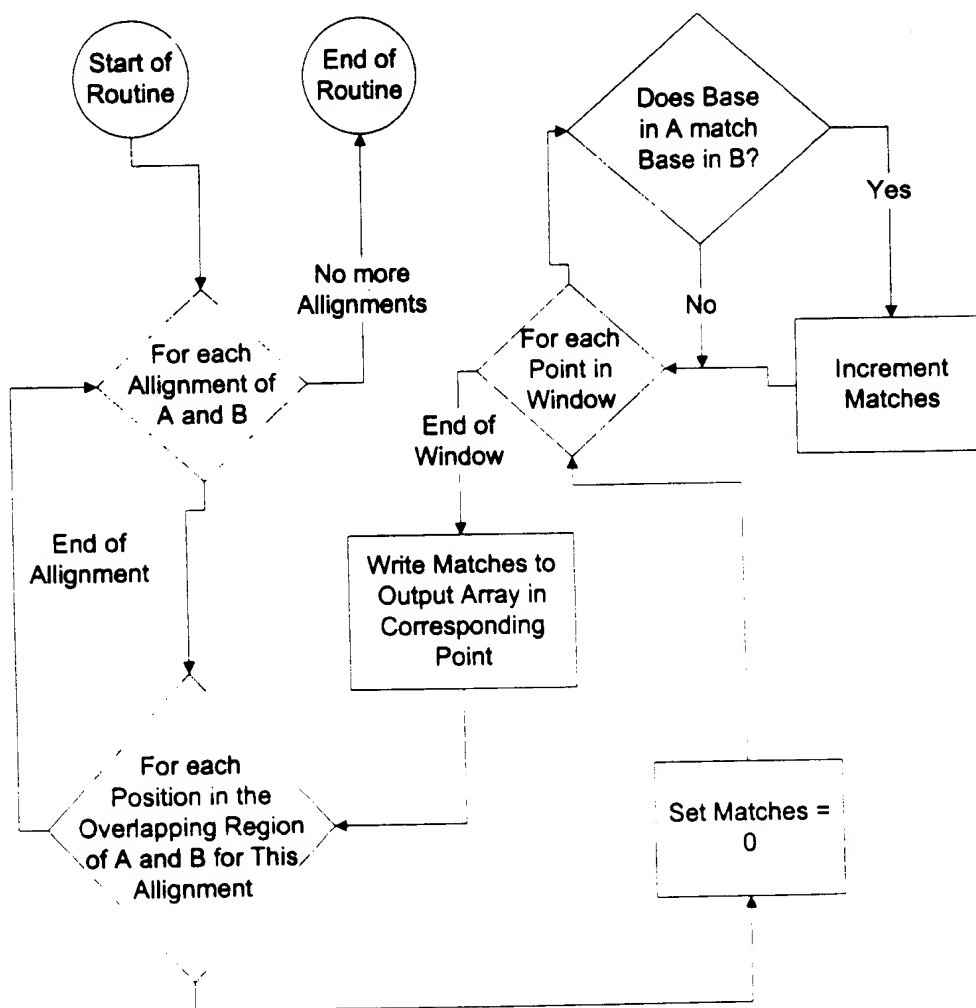
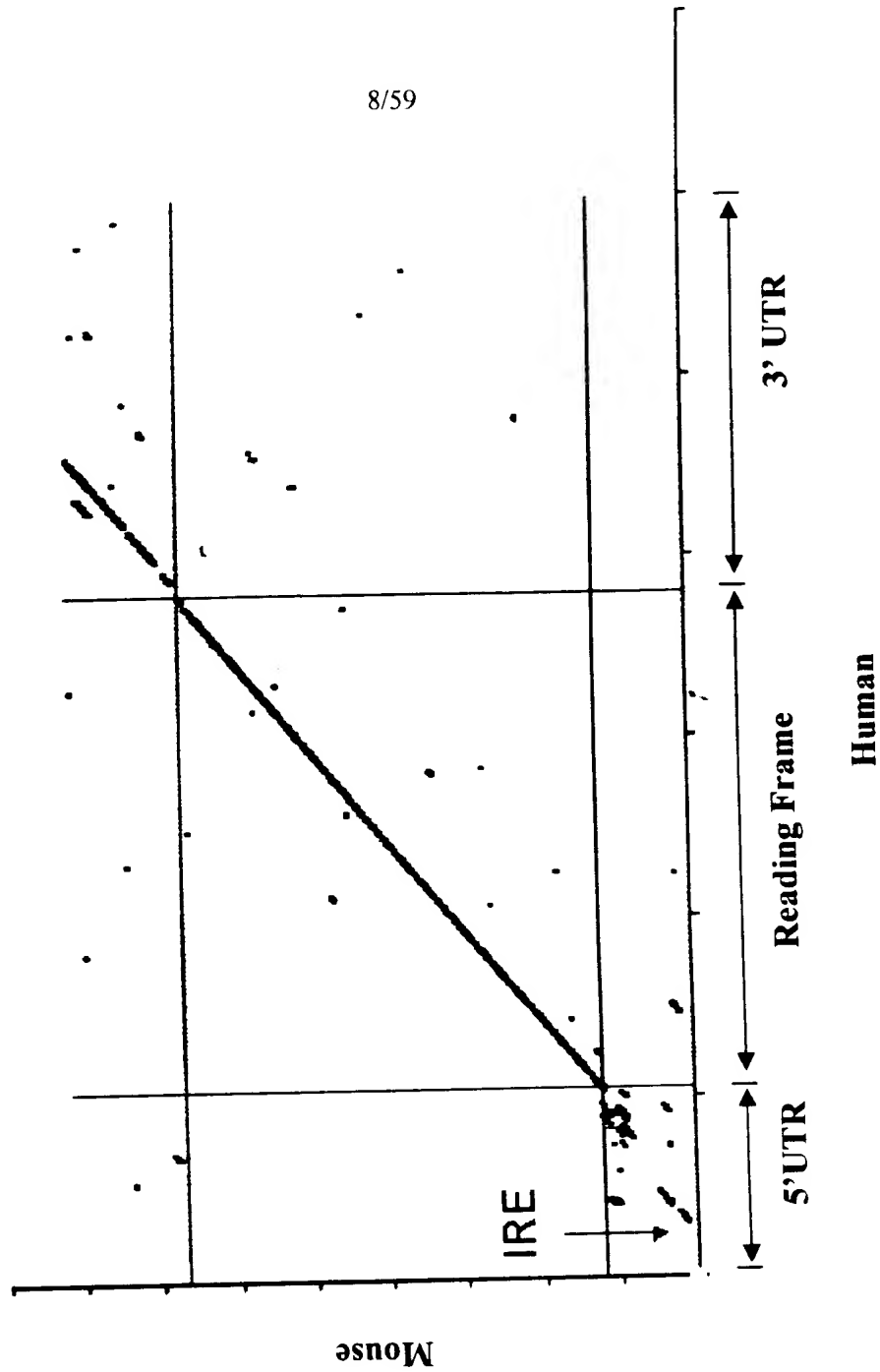


FIGURE 5C

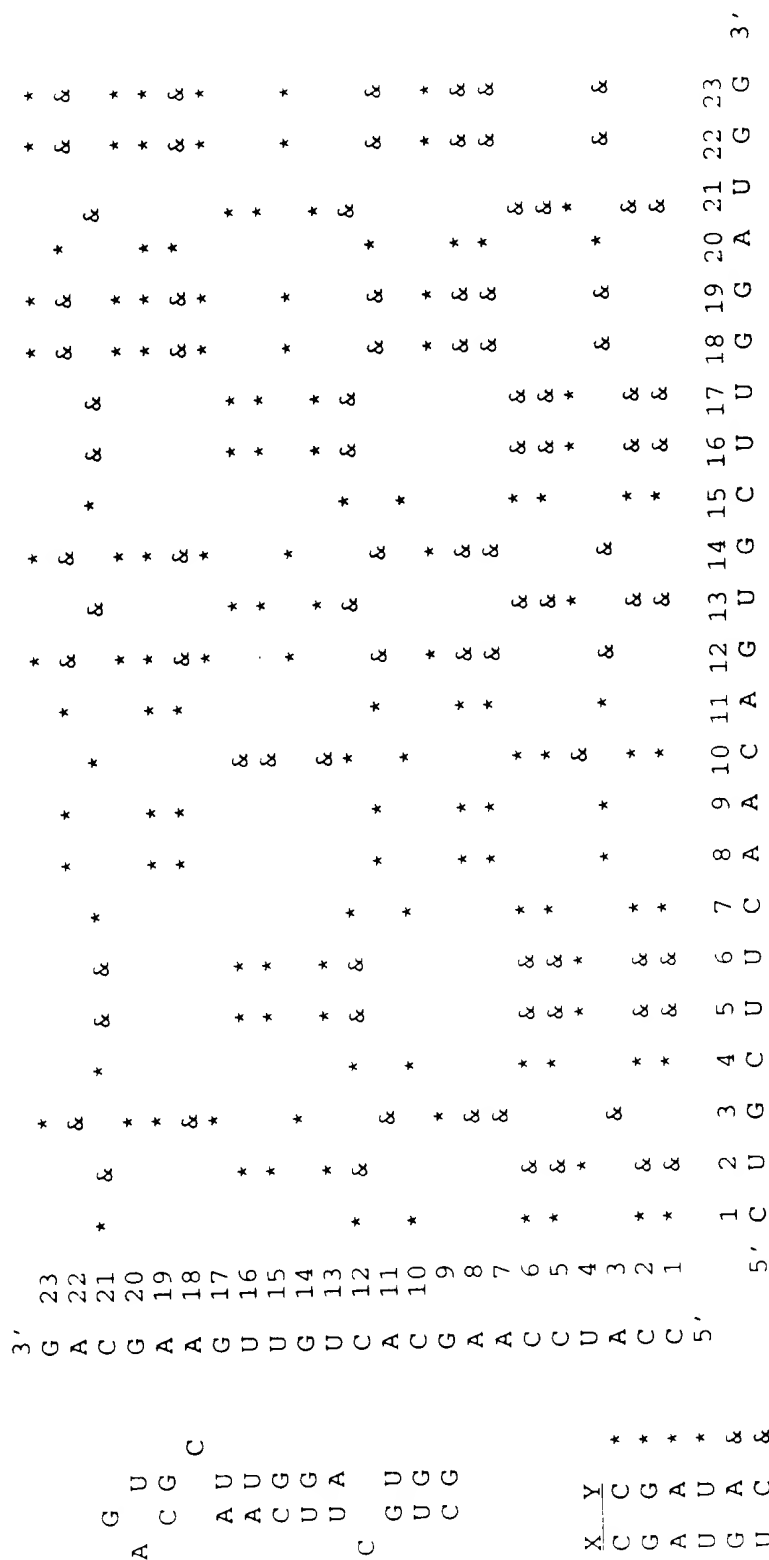
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Figure 6





## Self Complementation Analysis - Single Sequence

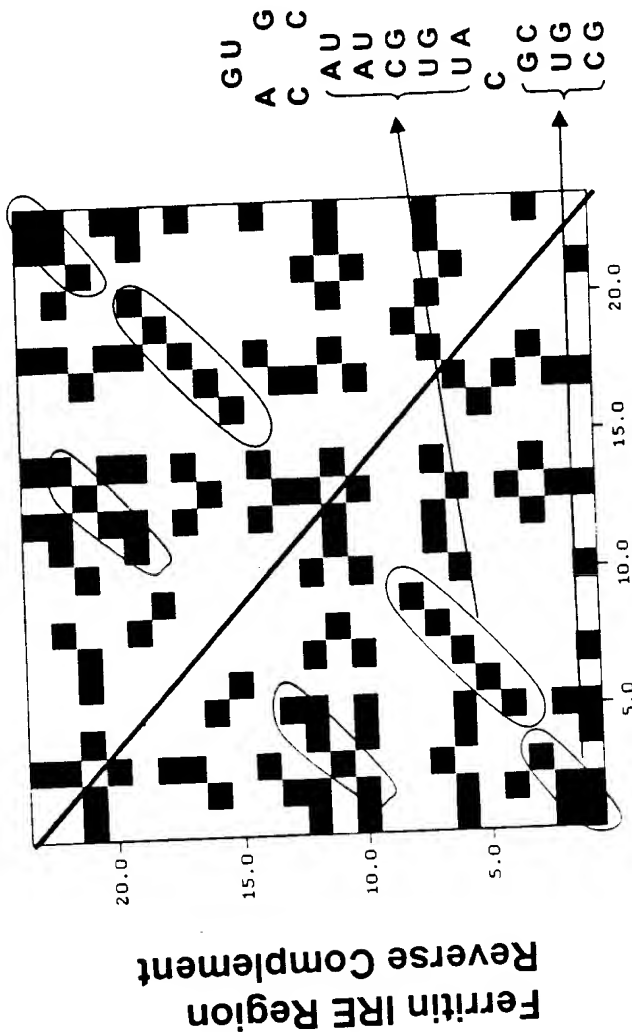


## Figure 7

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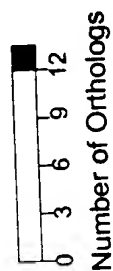
# Self Complementarity Comparisons

13 ortholog overlay



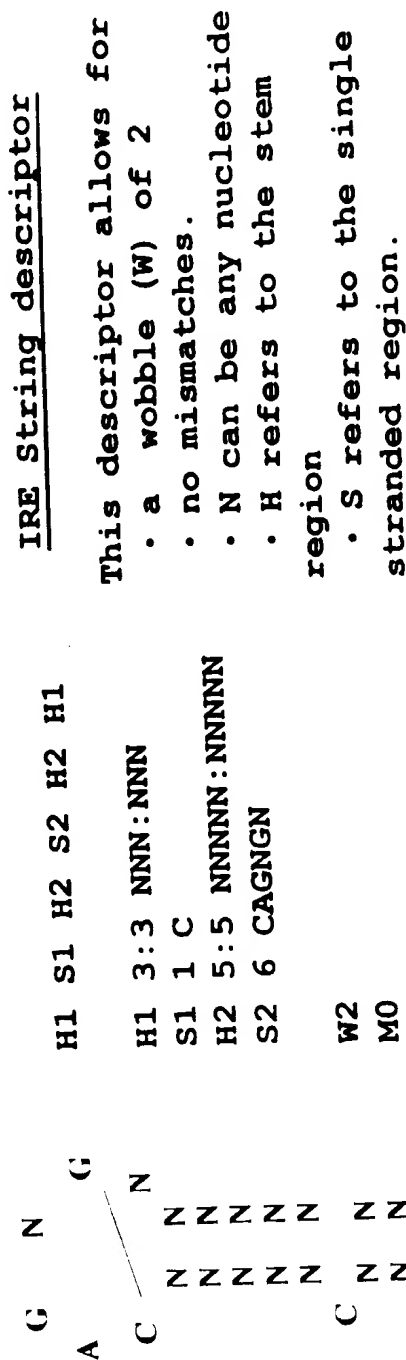
Ferritin IRE Region

Figure 8



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Figure 9



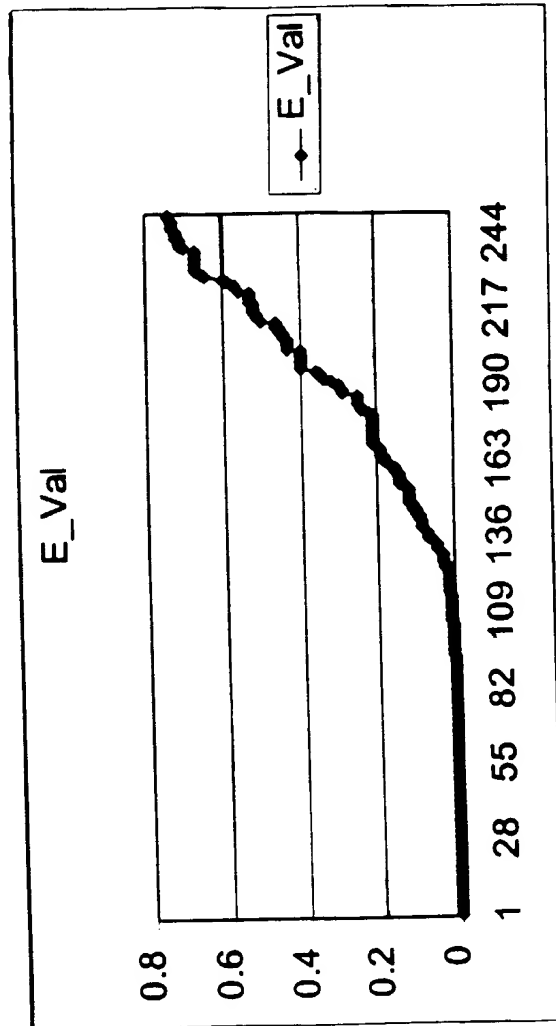
IRE String descriptor

This descriptor allows for

- . a wobble (W) of 2
- . no mismatches.
- . N can be any nucleotide
- . H refers to the stem region
- . S refers to the single stranded region.

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Figure 10



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Figure 11

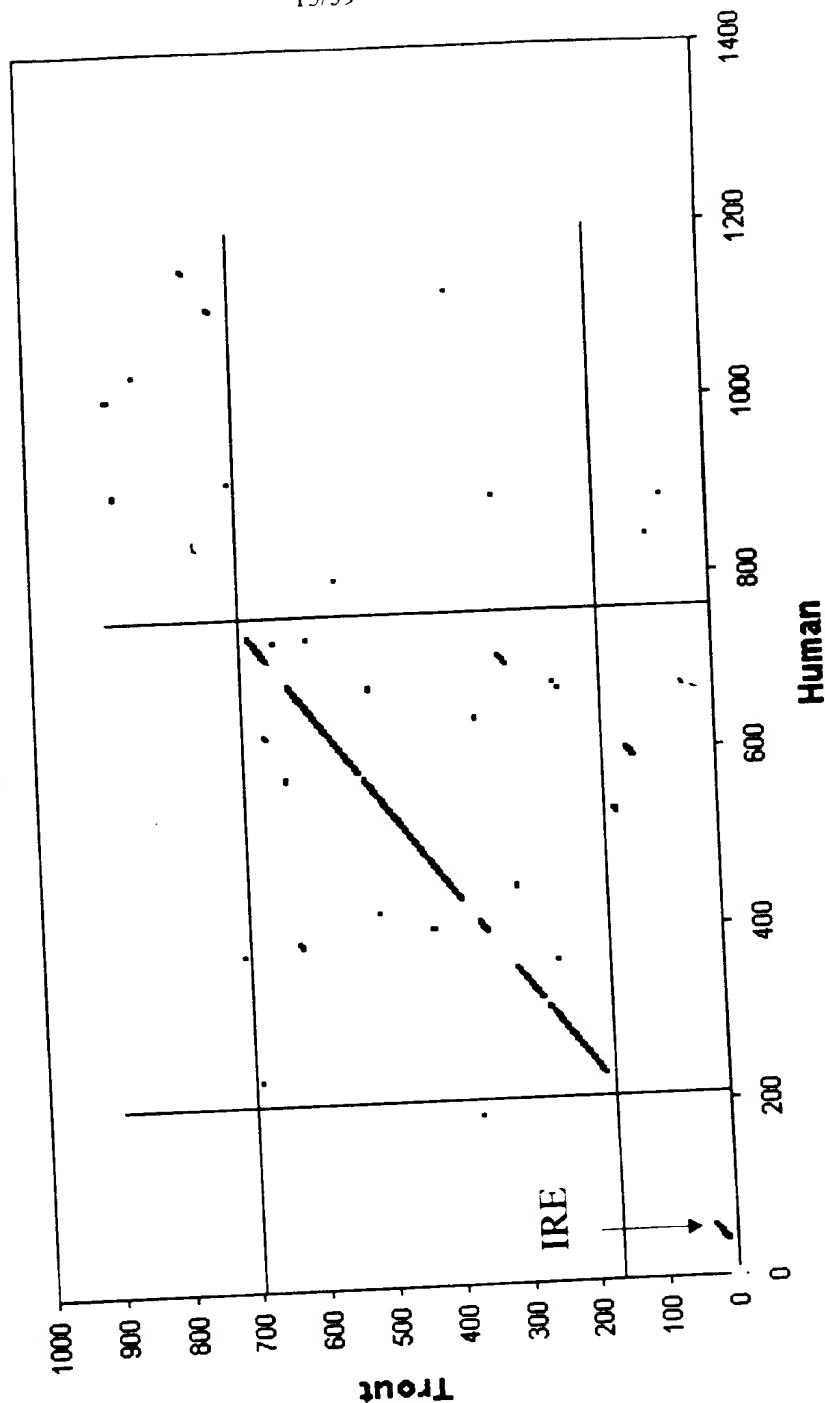
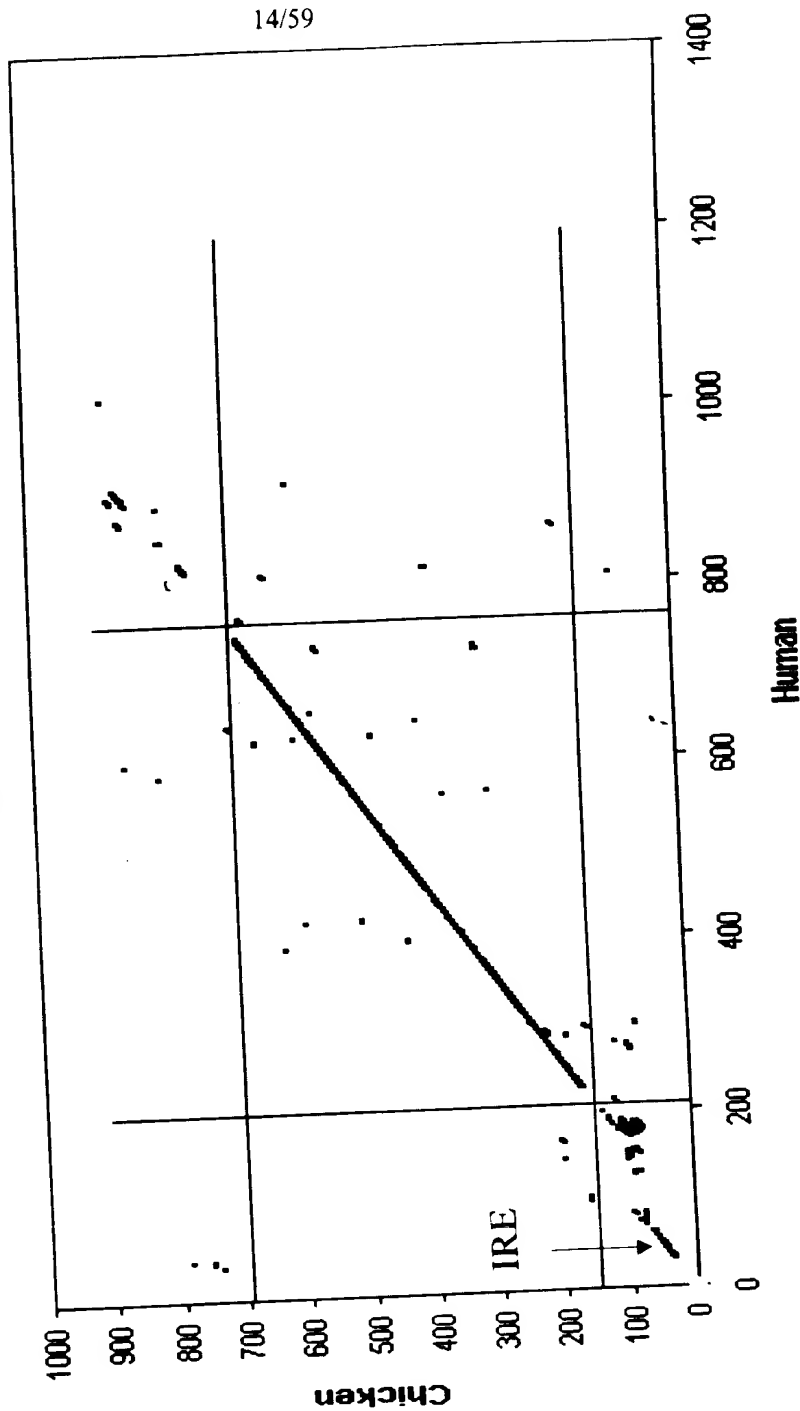


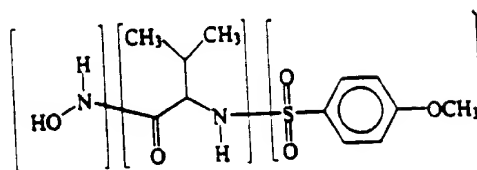
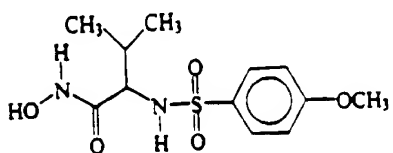
Figure 12



**Figure 13**

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Compound CI



	Fi	Fii	Fiii
Molecular formula	$H_2NO$	$C_3H_8NO$	$C_7H_7O_3S$

Figure 14



**Figure 15**

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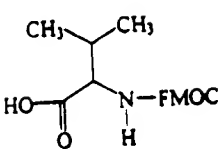
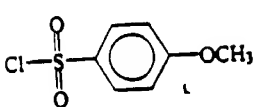
Reagents	Identifier	Name	Properties
$\text{H}-\text{O}-\text{NH}_2$ or $\text{P}-\text{O}-\text{NH}_2$	R <sub>i</sub>	Hydroxylamine	...
	R <sub>ii</sub>	FMOC blocked amino acid	...
	R <sub>iii</sub>	Sulfonylchloride	...
<p>Ⓟ = Solid support</p>			

Figure 16

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Transformation

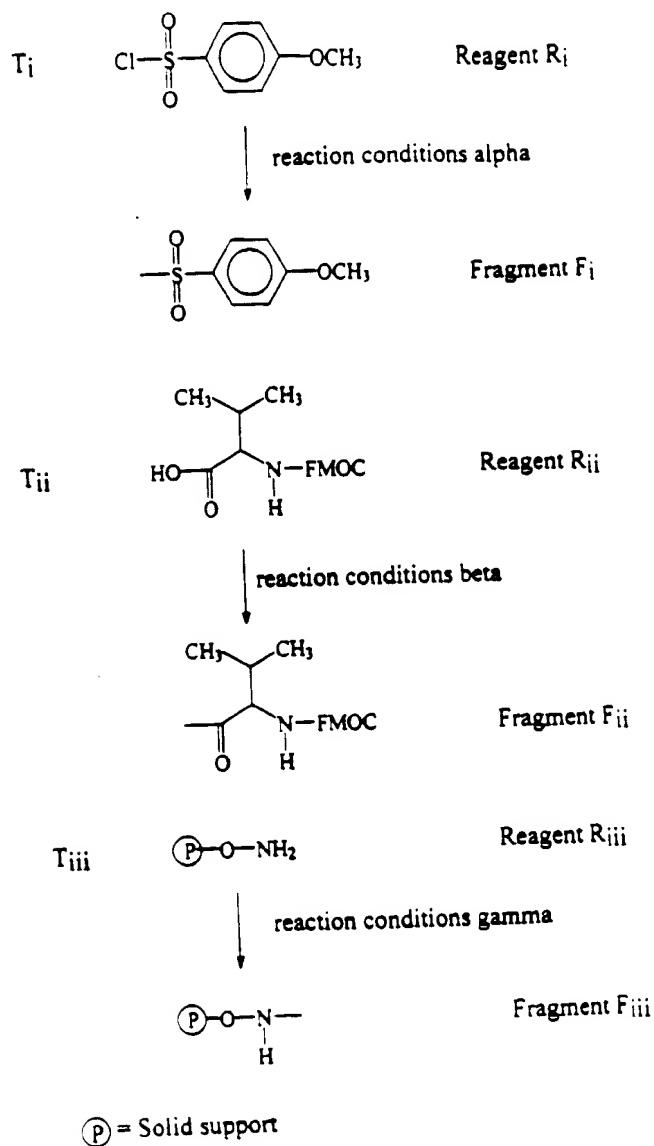


Figure 17

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Common Fragment / Different Reagents and Transformations

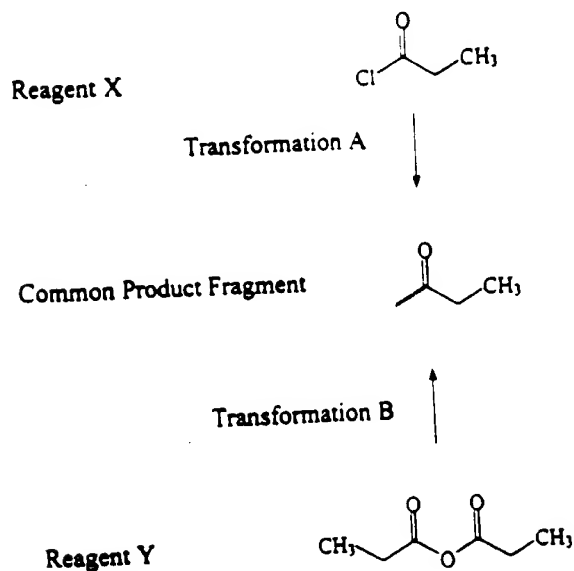


Figure 18

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Common Reagent

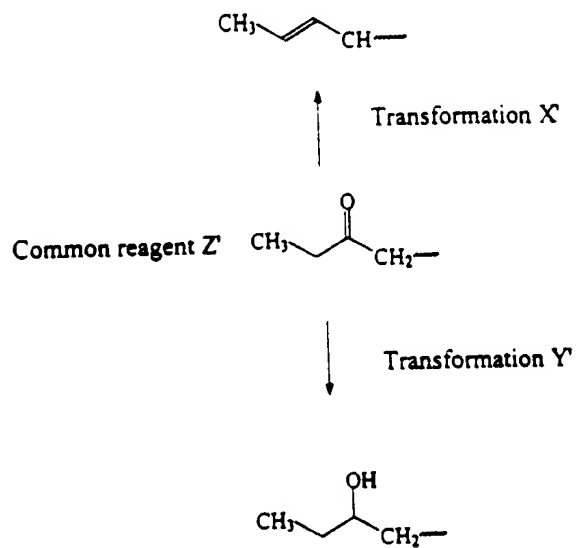


Figure 19B

<u>Symbolic Structure</u>	<u>Symbolic Identifier</u>	<u>Molecular formula</u>
---------------------------	----------------------------	--------------------------

Fi'

CuHvNw ...

$$O-X$$

Fii'

C<sub>u</sub>H<sub>v</sub>N<sub>w</sub> ...

$$X - \bigcirc - Y$$

Fiii'

C<sub>u</sub>H<sub>v</sub>N<sub>w</sub> ...

CT

CuHvNw ...

Molecular formula  $\text{F}_2$

+

Molecular formula F ii'

+

Molecular formula F iii'

= Molecular formula  $\text{Cl}^+$

**Figure 20**

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Symbolic Reagent Table


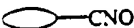

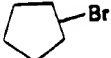
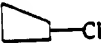
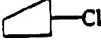
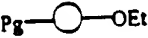
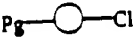

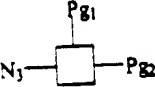
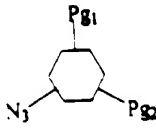
Identifier	Name	Structure	Molecular formula
R1	xxx		xxx
R2	...		...
R3	...		...
R4	...		...
R5	...	 	...
R6	...		...
R7	...		...
R8	...		...
R9	...		...
R10	...		...

Figure 21



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Symbolic Fragment Table






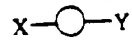

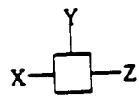
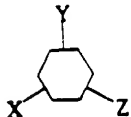
Identifier	Symbolic Structure	Molecular formula	Molecular Weight
F1		xxx	xxx
F2		...	...
F3		...	...
F4	 	...	...
F5		...	...
F6		...	...
F7		...	...
F8		...	...

Figure 22

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Symbolic Transformation Table


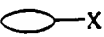
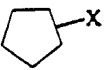

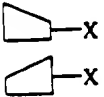

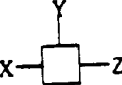
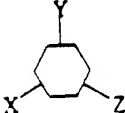
Identifier		Symbolic Reactions	Reagent
T1	F1	 $\xleftarrow{\quad}$ R1	conditions $\alpha$
T2	F2	 $\xleftarrow{\quad}$ R2	conditions $\beta$
T3	F3	 $\xleftarrow{\quad}$ R3	conditions $\alpha$
T4	F3	 $\xleftarrow{\quad}$ R4	conditions $\alpha$
T5	F4	 $\xleftarrow{\quad}$ R5	conditions $\alpha$
T6	F5	$X - \text{O} - Y$ $\xleftarrow{\quad}$ R6	conditions $\epsilon$
T7	F5	$X - \text{O} - Y$ $\xleftarrow{\quad}$ R7	conditions $\alpha$
T8	F6	 $\xleftarrow{\quad}$ R8	conditions $\alpha$
T9	F7	 $\xleftarrow{\quad}$ R9	conditions $\gamma$
T10	F8	 $\xleftarrow{\quad}$ R10	conditions $\gamma$

Figure 23

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# Single Compounds and Mixtures

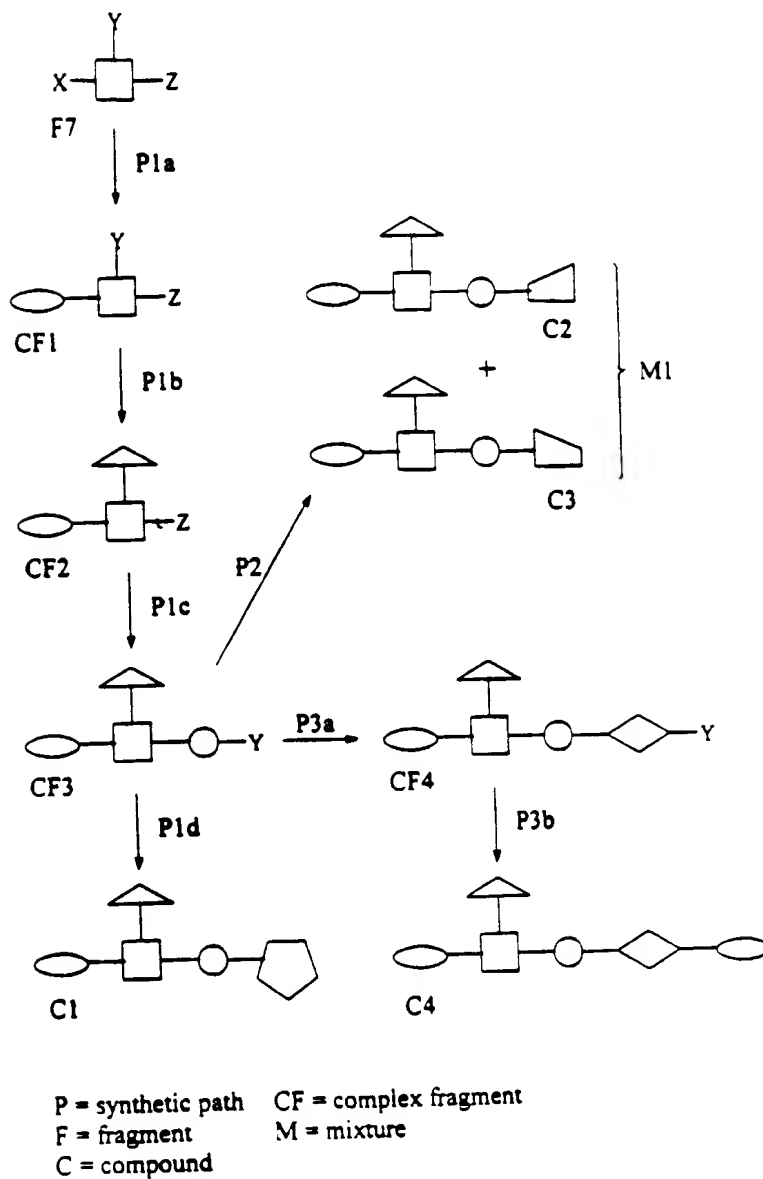


Figure 24

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Mixture 2

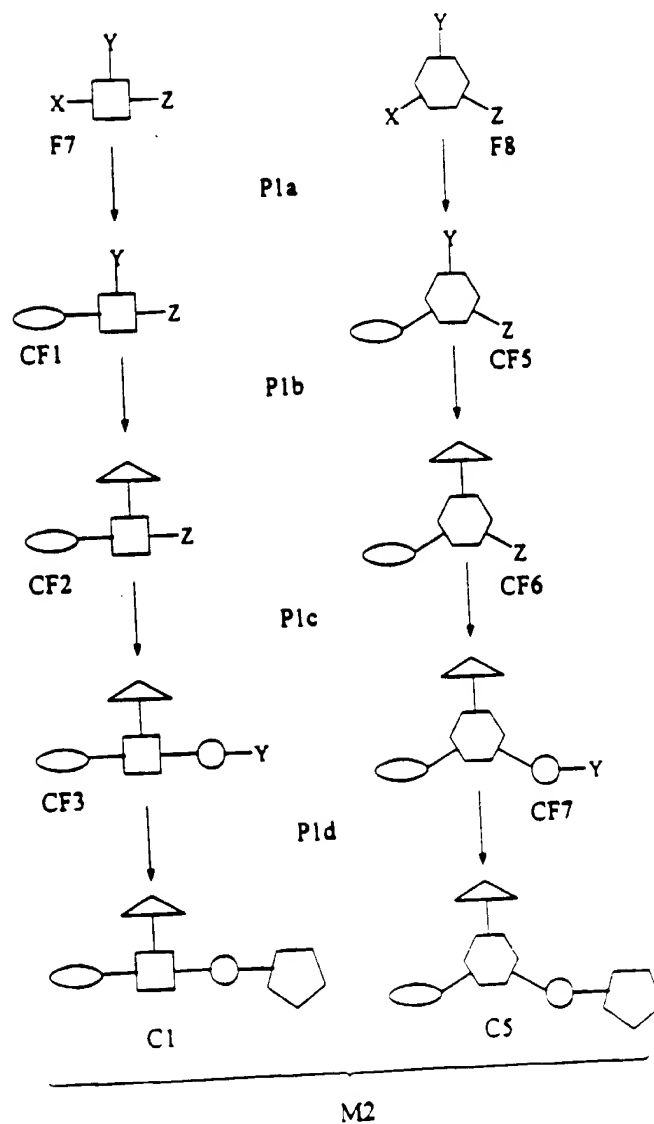
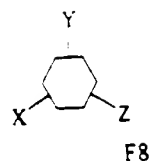
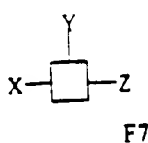


Figure 25

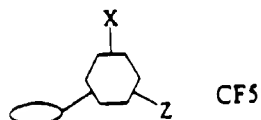
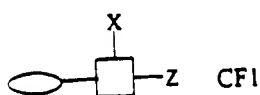
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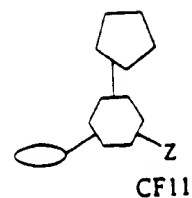
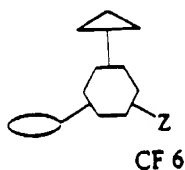
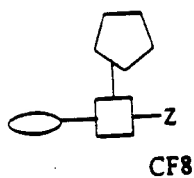
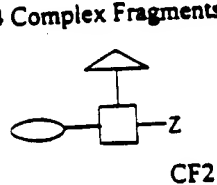
Mixture 4  
 2 Starting Fragments



2 Complex Fragments



4 Complex Fragments



8 Complex Fragments

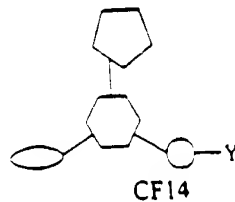
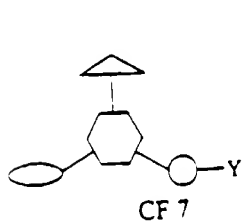
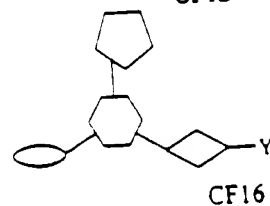
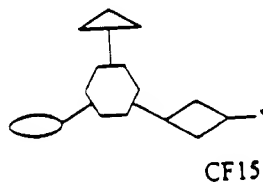
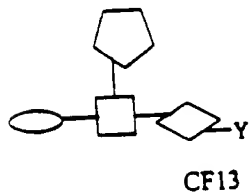
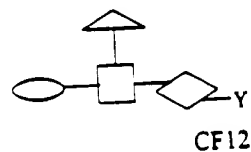
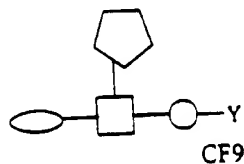
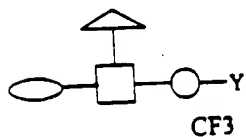


Figure 27A

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Mixture 4 (continued)

16 compounds

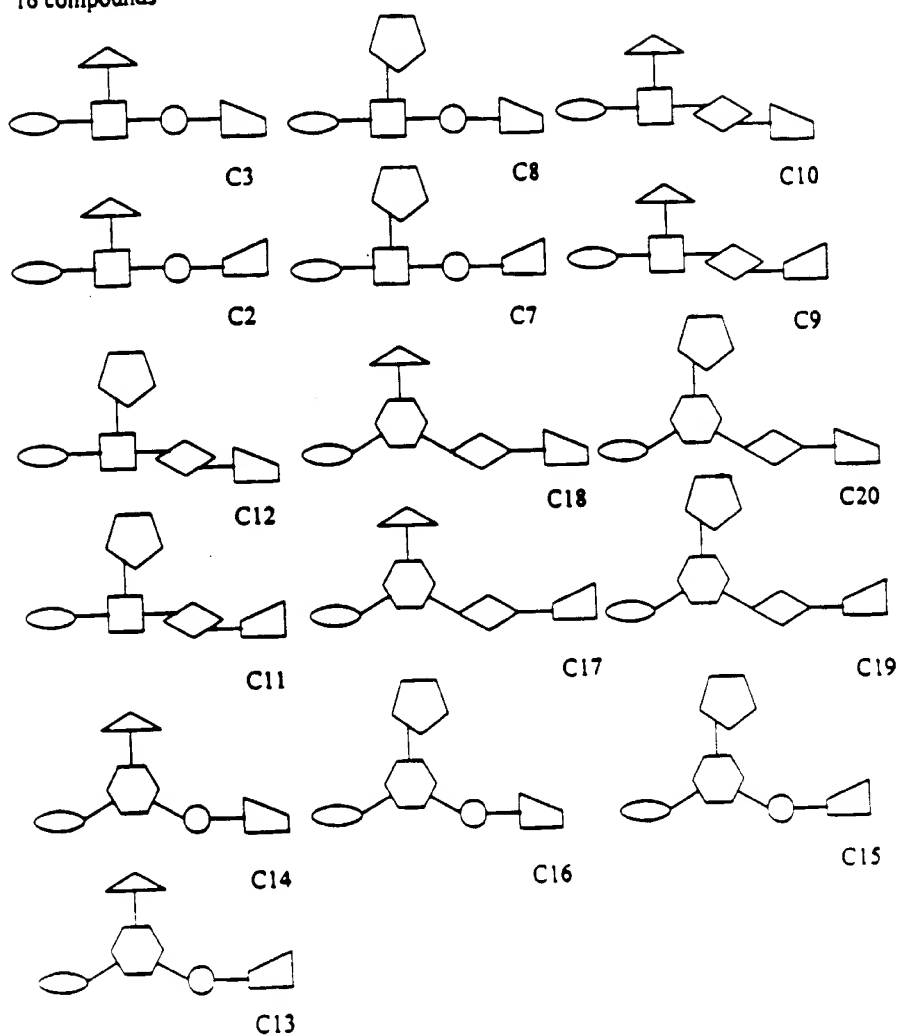


Figure 27B

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Tracking Table for Compound C1

(a) By Fragments:

n	n+1	n+2
F7	F2 F1 F5	F3

(b) By Transformations:

Synthesis Path 1

n	n+1	n+2
T9	T2 T1 T6	T3

Synthesis Path 2

n	n+1	n+2
T9	T2 T1 T7	T3

Synthesis Path 3

n	n+1	n+2
T9	T2 T1 T6	T4

Synthesis Path 4

n	n+1	n+2
T9	T2 T1 T7	T4

Figure 28



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# Tracking Table

## Tracking M1

### Step 1

T9		
----	--	--

### Step 2

T9	T2	
----	----	--

### Step 3

T9	T2 T1	
----	----------	--

### Step 4

T9	T2 T1 T7	
----	----------------	--

### Step 5

T9	T2 T1 T7	T5 <sup>1</sup>
----	----------------	-----------------

C2

### Step 5

T9	T2 T1 T7	T5 <sup>2</sup>
----	----------------	-----------------

C3

Figure 29

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# Tracking Table

## Tracking M2

Step 1		
n	n+1	n+2
T9		

Step 1		
n	n+1	n+2
T10		

Step 2		
n	n+1	n+2
T9	T2	

Step 2		
n	n+1	n+2
T10	T2	

Step 3		
n	n+1	n+2
T9	T2 T1	

Step 3		
n	n+1	n+2
T10	T2 T1	

Step 4		
n	n+1	n+2
T9	T2 T1 T7	

Step 4		
n	n+1	n+2
T10	T2 T1 T7	

Step 5		
n	n+1	n+2
T9	T2 T1 T7	T4

Step 5		
n	n+1	n+2
T10	T2 T1 T7	T4

C1

C5

Figure 30

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Tracking Table

Tracking M3

Step 1

T9		
----	--	--

Step 2

T9	T2	
----	----	--

Step 3

T9	T2	T1
----	----	----

Step 3

T9	T2	T3
----	----	----

Step 4

T9	T2	T1	T7
----	----	----	----

Step 4

T9	T2	T3	T7
----	----	----	----

Step 5

T9	T2	T1	T7	T5 <sup>1</sup>
				C2

Step 5

T9	T2	T1	T7	T5 <sup>2</sup>
				C3

Step 5

T9	T2	T3	T7	T5 <sup>1</sup>
				C7

Step 5

T9	T2	T3	T7	T5 <sup>2</sup>
				C8

Figure 31

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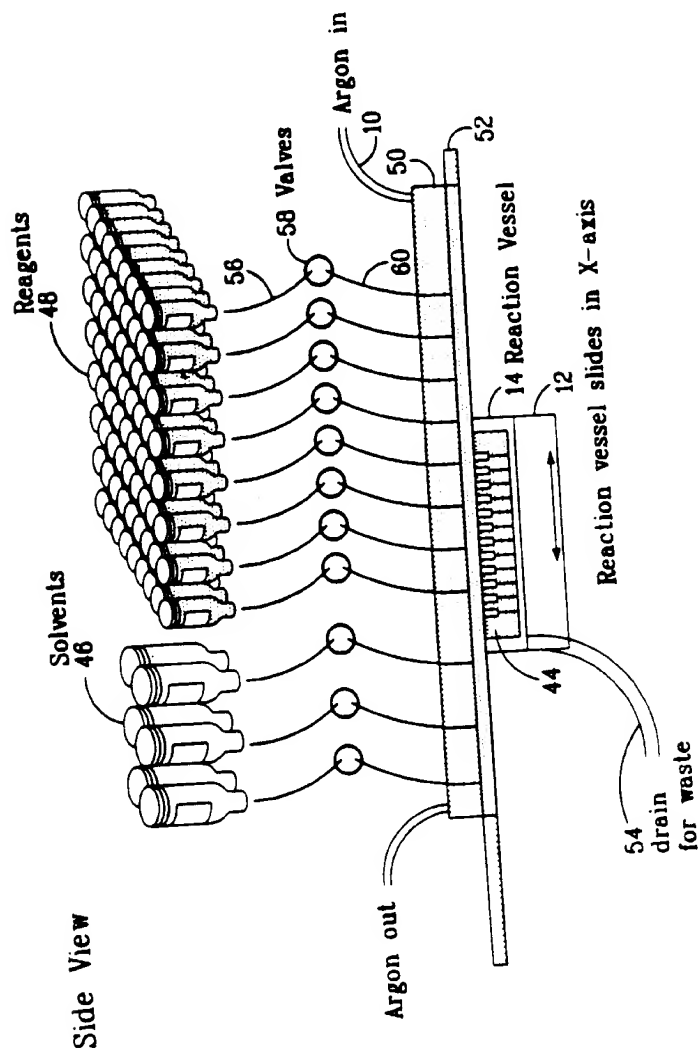


Figure 32

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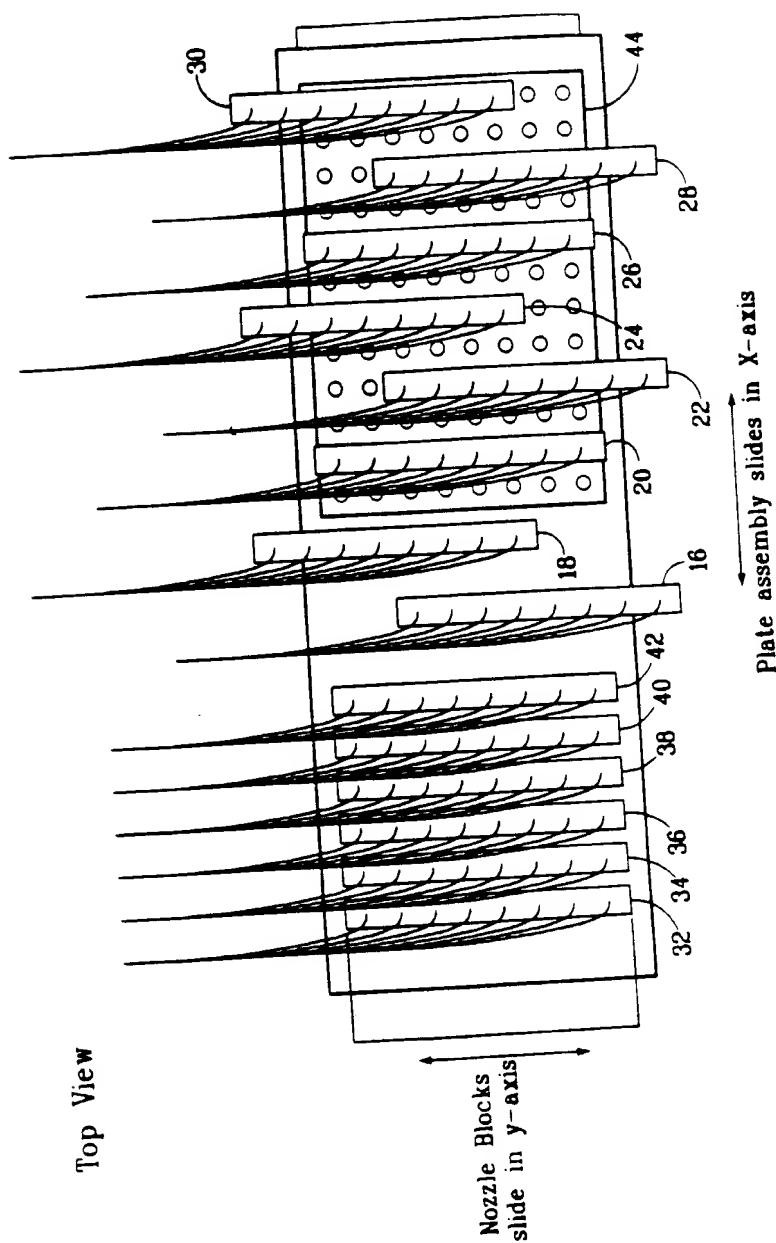


Figure 33

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Synthesis of hydroxamic acids from hydroxylamine resin

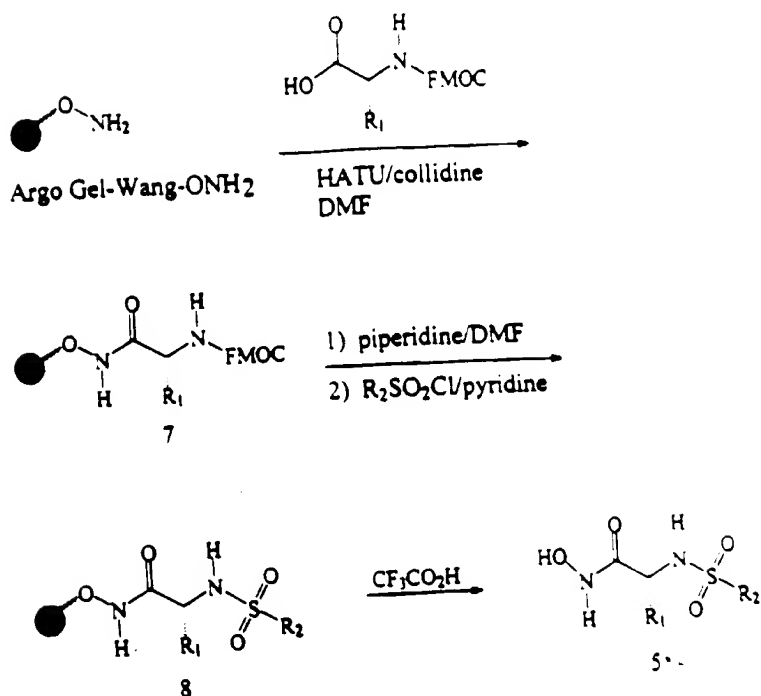
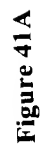


Figure 35







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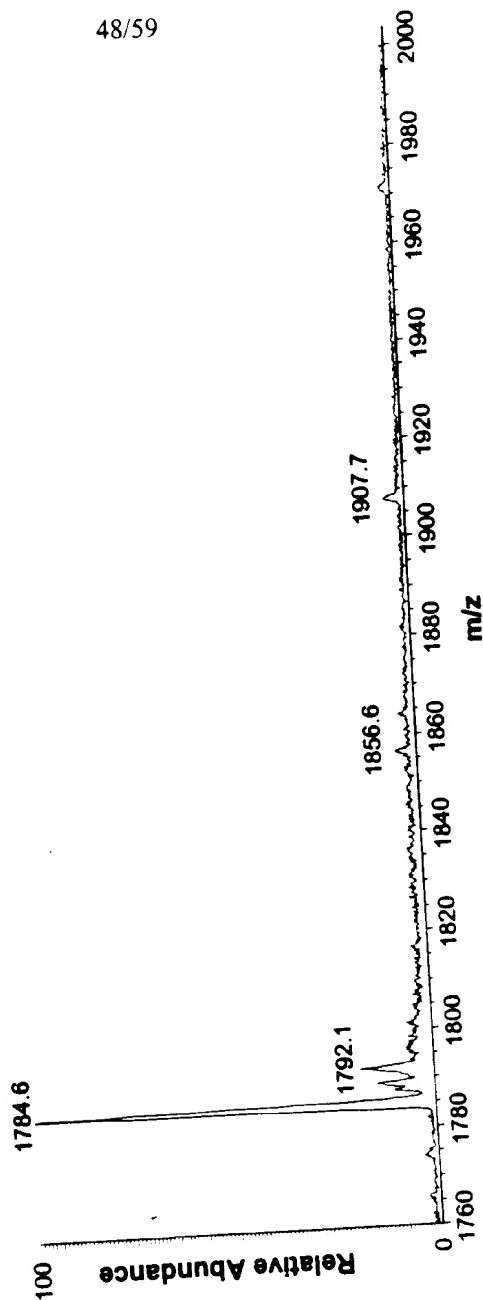


Figure 42A

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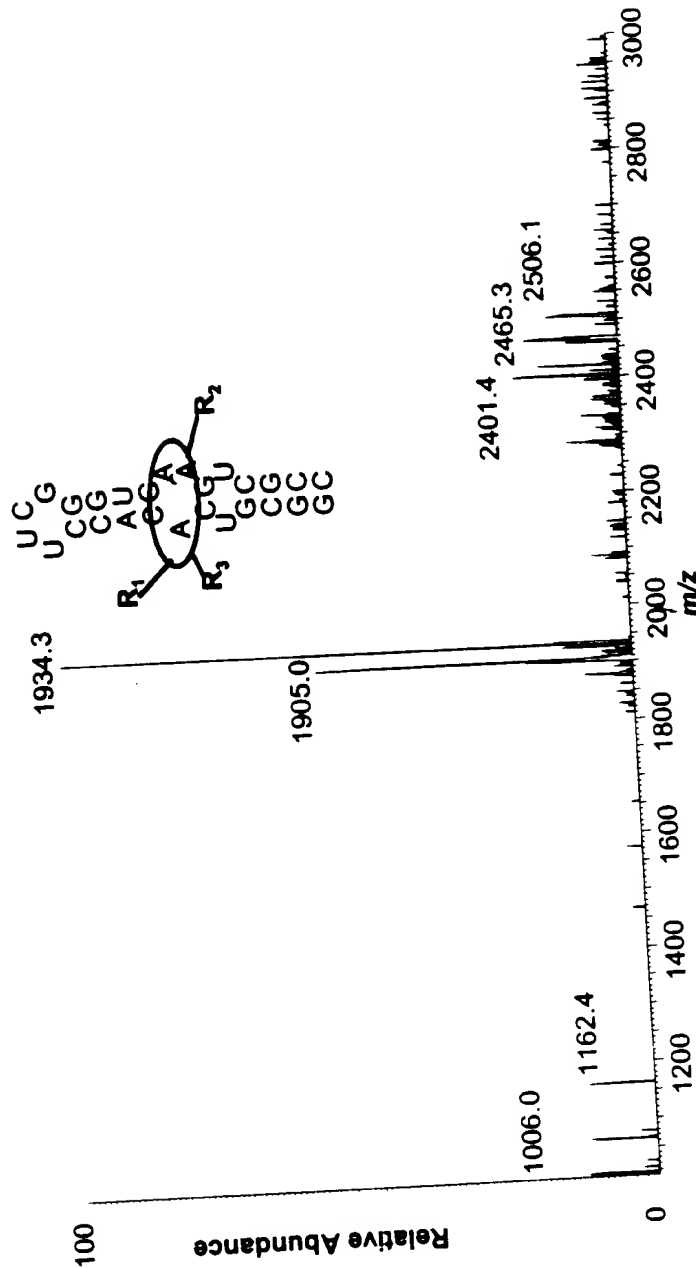
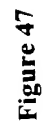


Figure 46





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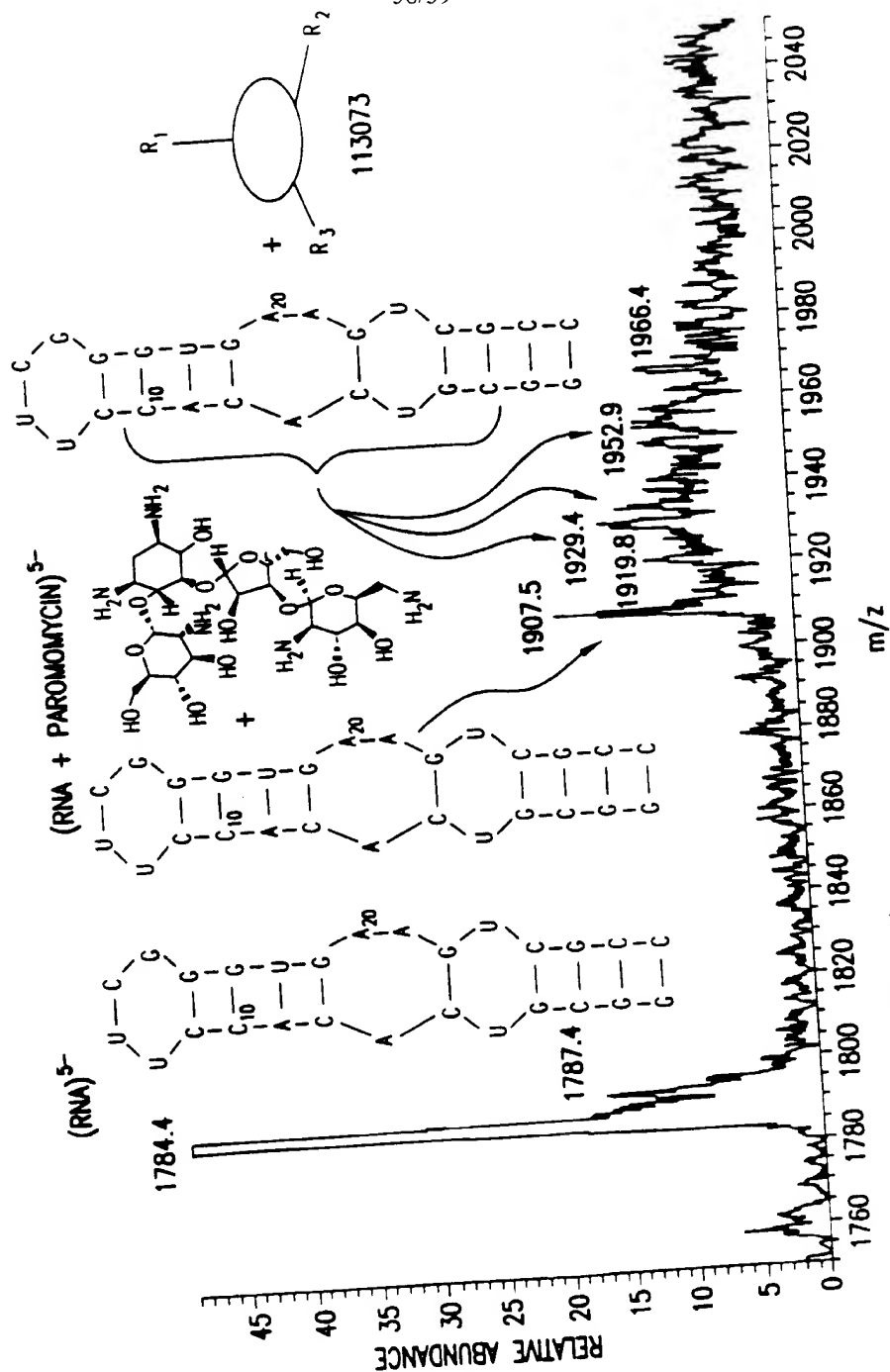


Figure 51

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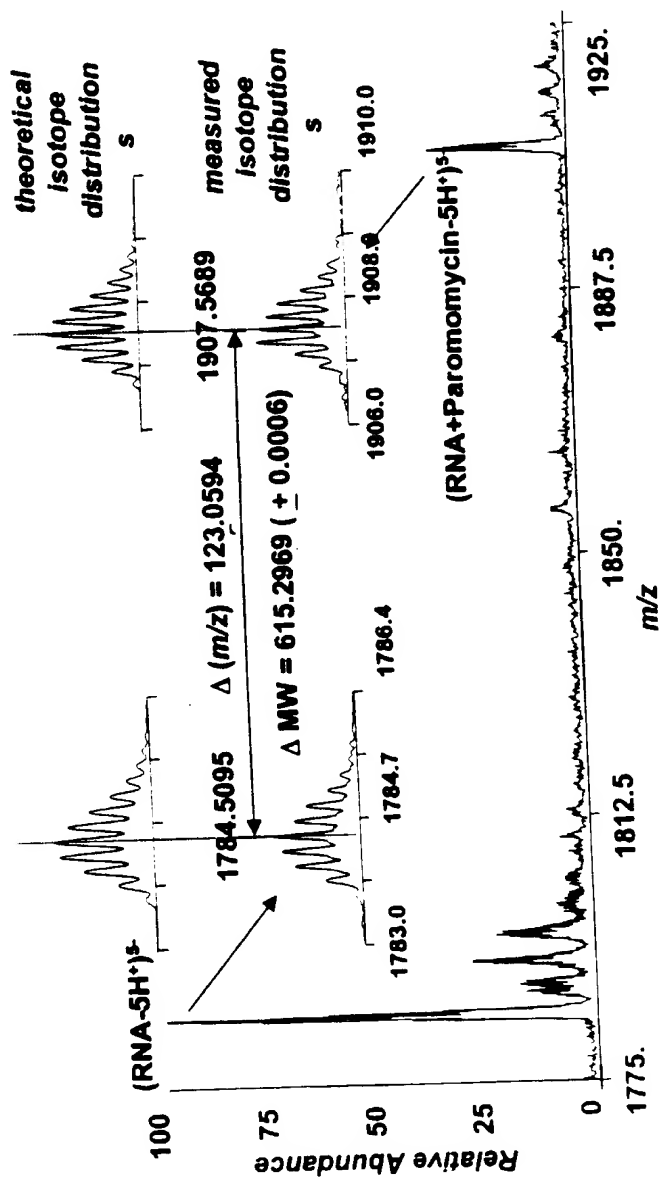


Figure 52